MODELING OF DIAMOND BASED DEVICES FOR BEAM DIAGNOSTICS*

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Abstract

Beamlines at new light sources, such as the National Synchrotron Light Source II will operate at flux levels beyond the saturation level of existing diagnostics, necessitating the development of new devices. Currently, there is no detector which can span the entire flux range that is possible even in a second generation light source and will become crucial for next generation light sources. One new approach [1] is a diamond-based detector that will be able to monitor beam position, flux and timing to much better resolution. Furthermore, this detector also has linear response to flux over 11 orders of magnitude. However, the successful development of the detector requires thorough understanding and optimization of the physical processes involved. We will discuss the new modeling capabilities we have been implementing in the VORPAL 3D code to investigate the effects of charge generation due to absorption of x-ray photons, transport, and charge trapping. We will report results from VORPAL simulations on charge collection and how it depends on applied field, charge trapping, and the energy of absorbed photons.

INTRODUCTION

Diamond has emerged as a promising candidate for development of improved beamline diagnostic devices. Synthetic single crystal diamond has several material properties (good thermal conduction, low Z (limiting absorption), and high mechanical strength) that are particularly important for applications in high-flux beam diagnostics for synchrotron beam lines and amplifiers for accelerator photo injectors. These technologically important material properties of diamond have been recognized and investigated for particle detectors [2] and now for high-flux beam monitors for synchrotron beamlines [3, 1]. They provide an opportunity for the development of diamond-based transmission beam monitors for next generation light sources and free electron lasers.

However, charge carrier transport in ultra-high purity synthetic diamond, particularly at high photon fluxes, is still to be properly understood to permit the development of diamond-based detectors with the desired performance characteristics. We have been implementing models for simulations [4], within the VORPAL particle-in-cell code (PIC), that describe the generation of secondary charge carriers produced by either electrons or x ray photons. However, in a real photon detector, collection efficiency, the role of trapped charge, impurities, surface effects need to be modeled as well. Such new modeling capabilities will allow investigation of collection efficiency, charge trapping, injection, time response in diamond as a function of photon energy, temperature, and applied electric field. Results from such simulations will be of importance to provide better understanding to design and develop diamond-based detectors for diagnostics optimization over material thickness, tolerance for defects, and need for clearing voltage.

Here, we discuss initial results from modeling trapping effects with VORPAL. We briefly describe the models we have implemented to simulate charge generation, transport, and trapping. Then, we report initial results on how collection efficiency in diamond depends on charge trapping, applied field, and energy of absorbed photons.

SIMULATION MODELS

We investigate an approach for simulating the response of diamond to x-ray photons with energies relevant for synchrotron beamline detectors. Specifically, we prototyped an algorithm to model collection efficiency from planar diamond detectors in current mode [3].

The measurement setup consists of a parallel plate detector of a given thickness with metal electrodes attached to opposite surfaces in order to apply external electric field. When a sufficiently energetic photon enters diamond, an electron-hole pair is created. Provided the electron and hole have sufficiently high energies (depending on the energy of the absorbed photon), they continue to create additional electron-hole (e-h) pairs via impact ionization. This process continues until the energies of the created free charge carriers become insufficient to produce new e-h pairs. The created free charge carriers move (via drift-diffusion) in applied electric field and scatter with phonons and charge impurities. If trapping centers are present in diamond, some experience trapping and detrapping events.

The current, in response to photon absorption, is measured from which the collected charge is determined. For the simulation studies here, we define the detector collection efficiency (CE) as the ratio of collected charge Q_c (due to electrons or holes) to the total charge Q_0 (again, electrons or holes) that *could* be generated by the ionizing photons: $\eta = Q_c/Q_0$. This definition underestimates the CE since the total Q_0 that could be generated, if the photons are absorbed in bulk diamond (or sufficiently inside diamond relative to the impact surface) is always greater (or

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equal) than the actual number of generated carriers that are created when some of the photons are absorbed close to the diamond impact surface. We calculate Q_0 by running simulations with the initial e-h pairs in bulk diamond. We are currently considering how to implement a more accurate algorithm for the calculation of Q_0.

In the simulations, we used our implementation of impact ionization for secondary electron and hole generation based on the Tanuma—Powell—Penn optical model. We model charge transport using the electron-phonon and hole-phonon scattering models we implemented and the VORPAL particle-push algorithm to advance charge particles in electro-magnetic fields. Our implementation of these models is described in Ref. [4].

For the simulations here, we implemented trapping and detrapping of electrons and holes. It is based on the model described by the equation:

$$\frac{\partial n_k}{\partial t} = -n_k \sum_{\alpha} \frac{v_k}{\lambda^T_{k,\alpha}} + \sum_{\beta} \frac{n^D_{k,\beta}}{\tau^D_{k,\beta}}, \qquad (1)$$

where n_k is the number of free particles of type k (electrons or holes), $n^D_{k,\beta}$ is the number of trapped particles at trapping centers of type β, $\lambda^T_{k,\alpha}$ is the mean free path for trapping due to trapping centers of type α, $\tau^D_{k,\beta}$ is the average detrapping time of trapping centers of type β and v_k is the drift velocity of k-type particles. We have implemented a Monte Carlo algorithm for this model that allows us to model arbitrary number of trapping/detrapping center types with the mean free paths and average detrapping times provided as input parameters to the code.

RESULTS

We present results from small-scale VORPAL simulations to start investigating how trapping and detrapping affect CE in diamond. The simulation domain (representing diamond) has lengths of $10.5 \times 19.2 \times 19.2$ μm (with $25 \times 46 \times 46$ total number of cells) along the x, y, and z axes, respectively. Similarly to the approach in the diamond detector experiments [1], we set up the simulations to maintain a given potential difference along the (x) length of the simulation domain using the feedback capability in VORPAL. We selected the potential difference such that a desired applied field in diamond is achieved.

We have set up the simulations with trapping in four phases. First, we run for 60000 time steps to establish the desired potential difference across the diamond simulation domain. We model diamond as a scalar dielectric using VORPAL's multi-field dielectric updater.

In the second phase, we introduce 100 e-h pairs, each with a total energy equal to the energy of absorbed photons. The distance of the e-h pairs from the diamond impact surface is sampled from an exponential distribution with parameters determined by the absorption length of photons in diamond with the considered energy. Transversely, the e-h pairs are distributed uniformly within a specified rectangular area (up to 0.5 the transverse length centered in the middle of the domain). The energies of each hole are uniformly sampled within the 23 eV valence band width. The energies of the electrons are then chosen to conserve energy given the initial energy of the photons. The directions of the initial momenta of electrons and holes are chosen randomly. The origin of time in the plots presented here is from the time e-h pairs are introduced in the simulation. The second phase is done with a time step of 8.33×10^{-17} s to resolve the impact ionization scattering rate. In this phase, sufficiently energetic electrons and holes generate additional e-h pairs. This phase is run for about 0.67 ps after which the existing free charge carriers practically do not have sufficient energy to generate additional e-h pairs. However, we consider that they are still energetic to be trapped (they have energies ~ 1 eV). Thus, in the third phase we run with only phonon scattering enabled and no trapping until the energies of these charge carriers are relaxed to their drift state energies of the order of 0.1 eV. We run this phase for 4.5 ps. Then, we switch on trapping/detrapping for the final phase of the simulations (with phonon scattering still on). Except for the second phase, a time step of 7.55×10^{-16} s is used. We have started to investigate the effect of trapping on CE with only one type of trapping centers for holes and one for electrons represented in the model given by Eq. (1). In the latter case, we also considered two different average detrapping times. The trapping parameters we used for electrons and holes are given in Table 1. The trapping mean free paths are similar to values from previous work [2] on studying trapping effects in diamond. We used smaller detrapping times to explore the resulting effects in a shorter time-scale simulations.

Table 1: Mean free paths for trapping and average detrapping times of electrons and holes that we used in the simulations.

Parameter	Symbol	Value	Unit
eletcron trapping MFP	λ^T_e	13.5	μm
ave. electr. detrapping time	τ^D_e	1 or 10	ns
hole trapping MFP	λ^T_h	30	μm
ave. hole detrapping time	τ^D_h	0.01	ns

We compare the effects of trapping and detrapping on CE (all values in %) to results from simulations without trapping (shown in Fig. 1 for both electrons and holes at 1.5 MV/m). The energy of absorbed photons was 600 eV for the results presented in Figs. 1 to 3 (Fig. 3 also contains results for 1 keV photons). At this applied field, electrons have drift velocity of about 1.3×10^5 m/s that is higher than for holes [4]. Thus, electron CE reaches saturation faster than the CE of holes at this field. Note that in our initial distribution of e-h pairs we have pairs created as deep as about 1.8 μm from the diamond photon impact surface.

In Fig. 2, we present results for CE of electrons at two

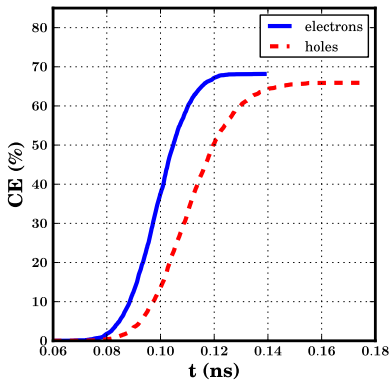

Figure 1: The CE of electrons without trapping reaches saturation values faster than the CE for holes at 1.5 MV/m applied field. Electrons have higher drift velocity than holes at this field.

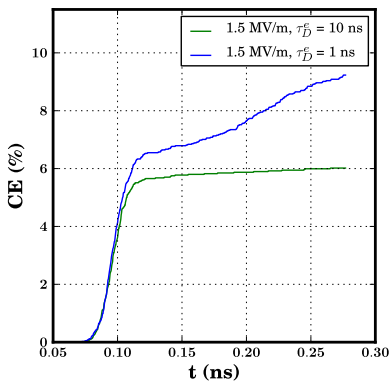

Figure 2: Increasing the detrapping time constant (for CE of electrons here), leads to increased number of trapped carriers and decreased CE vs time values.

different detrapping time constants. As expected, trapping strongly affects the observed CE vs time behavior compared to the case without trapping given in Fig. 1. The initial rise of the CE is due to electrons reaching the collection electrode before being trapped. The smaller slope of the CE rise after that time is due to collection of detrapped electrons.

We plot results on the dependence of the electron CE vs time for three different applied field values and for 600 eV and 1 keV photons in Fig. 3. Decreasing the applied field leads to decreasing the electron drift velocity and thus lower values of the measured CE at a given time. Increasing the energy of impacting photons, leads to creation of e-h pairs deeper in diamond leading to smaller initial time to start collecting electrons and increased CE at same applied fields. These initial results show the importance of including trapping and detrapping when modeling CE in diamond and indicate that it has to be taken into account when attempting to compare to experimental data.

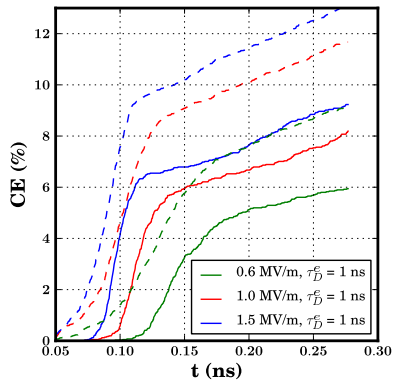

Figure 3: The CE can be increased when increasing the applied field at given trapping/detrapping parameters. The solid lines are for 600 eV photons, while the dashed are for 1 keV.

SUMMARY

We reported here initial simulation results for CE of diamond when trapping and detrapping are taken into account. We consider that our implementation in VORPAL of trapping and detrapping is working properly since the behavior we observed in the CE vs time is similar to results from previous experimental and simulation studies [2]. In future work, we are considering the implementation of a more accurate algorithm for measuring CE in the simulations that is based on Shockley-Ramo's theorem (see, e.g. Ref. [5]) when applied to semiconductor detectors. Moreover, we expect that modeling of diamond-metal contacts (ohmic and blocking) will be important to include in order to properly account and understand the experimentally observed CE data.

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